

Single-step controlled-NOT logic from any exchange interaction

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A self-contained approach to studying the unitary evolution of coupled qubits is introduced, capable of addressing a variety of physical systems described by exchange Hamiltonians containing Rabi terms. The method automatically determines both the Weyl chamber steering trajectory and the accompanying local rotations. Particular attention is paid to the case of anisotropic exchange with tracking controls, which is solved analytically. It is shown that, if computational subspace is well isolated, any exchange interaction can always generate high-fidelity, single-step controlled-NOT (CNOT) logic, provided that both qubits can be individually manipulated. The results are then applied to superconducting qubit architectures, for which several CNOT gate implementations are identified. The paper concludes with consideration of two CNOT gate designs having high efficiency and operating with no significant leakage to higher-lying non-computational states.

I. INTRODUCTION

Controllability of quantum mechanical systems has been the subject of numerous investigations in the last several years [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. An important contribution by Khaneja et al. on time-optimal control [3, 7] has led to the development of rf-pulse sequences for NMR-spectroscopy with nearly ideal performance [12]. In Refs. [3] and [7] it was assumed that the local terms in the Hamiltonian can be made arbitrarily large, which would allow an almost instantaneous execution of single-qubit operations. However, such hard control mechanism is not applicable to quantum computing architectures based on superconducting Josephson devices, in which the relevant computational subspace must be kept well isolated at all times.

In this regard, the work of Zhang et al. on geometric theory of nonlocal two-qubit operations [13, 14] acquires special significance. The authors introduced a convenient, geometrically transparent description of $SU(4)$ local equivalence classes and then used it to develop several implementations of quantum logic gates that did not involve hard-pulse control sequences. The description of entangling operations presented in Refs. [13] and [14] is based on the fact [3, 7] that any two-qubit quantum gate $U \in U(4)$ can always be written as a product, called the *Cartan decomposition*,

$$U = e^{i\varphi} k_1 U_{\text{ent}} k_2, \quad k_1, k_2 \in SU(2) \otimes SU(2), \quad (1)$$

with

$$U_{\text{ent}} = e^{-(i/2)(c_1 \sigma_1^x \sigma_2^x + c_2 \sigma_1^y \sigma_2^y + c_3 \sigma_1^z \sigma_2^z)}. \quad (2)$$

The triplet of numbers $\vec{c} = (c_1, c_2, c_3)$ in Eq. (2) may be taken to represent the local class of U . In general, such representation is *not* unique due to the presence of symmetries mapping class vectors to other class vectors of the same equivalence class. However, it was shown in [13] that the correspondence *can* be made unique if \vec{c} is restricted to a tetrahedral region of \mathbb{R}^3 , called a Weyl chamber. One such chamber is chosen to be canonical. It is described by the following three conditions [13, 15]:

- (i) $\pi > c_1 \geq c_2 \geq c_3 \geq 0$,
- (ii) $c_1 + c_2 \leq \pi$,
- (iii) if $c_3 = 0$, then $c_1 \leq \pi/2$.

When a physical system evolves under the action of its Hamiltonian, \vec{c} traces a trajectory inside the Weyl chamber, which explicitly shows the (continuous) sequence of dynamically generated local equivalence classes. For example, the Hamiltonian $H = g\sigma_1^x \sigma_2^x/2$ generates the straight line $\vec{c}(t) = (gt, 0, 0)$ in the Weyl chamber. In *this* case, Eq. (1) reduces to

$$U(t) = e^{-itH} \equiv U_{\text{ent}}(t), \quad k_1, k_2 = 1. \quad (3)$$

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After steering for a time $t_{\text{CNOT}} = \pi/2g$ the system hits the gate

$$U(t_{\text{CNOT}}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -i \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ -i & 0 & 0 & 1 \end{pmatrix}, \quad (4)$$

with

$$\vec{c} = \pi/2 \times (1, 0, 0), \quad (5)$$

belonging to the controlled-NOT equivalence class. By flanking $U(t_{\text{CNOT}})$ with additional local rotations K_1 and K_2 , any gate in that class can be made. For example, to make the *canonical* CNOT gate we can take

$$\text{CNOT} = e^{i\pi/4} \underbrace{e^{-i(\pi/4)\sigma_1^y} e^{i(\pi/4)(\sigma_1^x - \sigma_2^x)}}_{K_1} U(t_{\text{CNOT}}) \underbrace{e^{i(\pi/4)\sigma_1^y}}_{K_2}. \quad (6)$$

When Rabi terms are present in the Hamiltonian, the steering trajectory is no longer a straight line. In Ref. [13], the trajectory $\vec{c}(t)$ was calculated using the relation between the class vectors and the local invariants [16]. That method was applied in Ref. [17] to a CNOT gate design for flux-qubits with SQUID-based controllable coupling.

In the present paper we propose an alternative approach to finding the steering trajectory that does not rely on local invariants. Our goal is to develop a systematic procedure for calculating the entangling part $U_{\text{ent}}(t)$ of the time-dependent gate $U(t)$ together with the accompanying local rotations $k_1(t)$ and $k_2(t)$, so that the Cartan decomposition (1) could be determined at every step of system's evolution. It turns out that due to a special property of the relevant to our problem generators of $\mathfrak{su}(4)$ — the closure under commutation and the existence of a central element — the local rotations required to implement (1) can be chosen in a particularly simple form, which mimics the form of the local Rabi parts of system's Hamiltonian. Due to such simplifying form of k_1 and k_2 , the full problem of steering can be analytically solved in the experimentally important case of tracking control.

In the mathematical portions of this paper we will use the notation that is convenient for Lie algebraic manipulations:

$$X_k = (i/2)\sigma_k^x, \quad XX = (i/2)\sigma_1^x\sigma_2^x, \quad YY = (i/2)\sigma_1^y\sigma_2^y, \quad ZZ = (i/2)\sigma_1^z\sigma_2^z, \quad YZ = (i/2)\sigma_1^y\sigma_2^z, \quad ZY = (i/2)\sigma_1^z\sigma_2^y, \quad (7)$$

with $k = 1, 2$. The operators listed above form the Lie algebra $L_0 = \text{span}\{X_1, X_2, XX, YY, ZZ, YZ, ZY\} \subset \mathfrak{su}(4)$ whose commutators are given in the following table:

	X_1	X_2	XX	YY	ZZ	YZ	ZY
X_1	0	0	0	$-ZY$	YZ	$-ZZ$	YY
X_2	0	0	0	$-YZ$	ZY	YY	$-ZZ$
XX	0	0	0	0	0	0	0
YY	ZY	YZ	0	0	0	$-X_2$	$-X_1$
ZZ	$-YZ$	$-ZY$	0	0	0	X_1	X_2
YZ	ZZ	$-YY$	0	X_2	$-X_1$	0	0
ZY	$-YY$	ZZ	0	X_1	$-X_2$	0	0

(8)

Later on, in sections devoted to applications, we will revert to the usual notation.

Notice that it is possible to generate Lie algebras isomorphic to (8) by replacing the local operators (X_1, X_2) with either (Y_1, Y_2) or (Z_1, Z_2) , without any change in our results. An example of this will be given in Sec. III C 3.

II. GENERAL CONSIDERATIONS

Let us consider a generic time-dependent Hamiltonian

$$iH(t) = \Omega_{1x}(t)X_1 + \Omega_{2x}(t)X_2 + g_{xx}(t)XX + g_{yy}(t)YY + g_{zz}(t)ZZ + g_{yz}(t)YZ + g_{zy}(t)ZY, \quad (9)$$

whose scalar functions will be called the *steering controls*, or *control parameters*. The solution to the Schrödinger equation

$$\frac{dU(t)}{dt} = -iH(t)U(t), \quad U(0) = 1, \quad (10)$$

is a time-dependent operator $U(t) \in \exp(L_0) \subset \text{SU}(4)$, which can always be written in the form [18]

$$U(t) = \underbrace{e^{-\alpha(t)X_1 - \beta(t)X_2}}_{k_1(t)} \underbrace{e^{-c_1(t)XX - c_2(t)YY - c_3(t)ZZ}}_{U_{\text{ent}}(t)} \underbrace{e^{-\zeta(t)X_1 - \xi(t)X_2}}_{k_2(t)}. \quad (11)$$

The functions appearing in the exponents of Eq. (11) will be collectively referred to as the *steering parameters*, while the triplet $(c_1(t), c_2(t), c_3(t))$ will be called the *class vector*, as usual [15]. In what follows, the class vector will be allowed to evolve on the full Cartan subalgebra $A_C = \text{span}\{XX, YY, ZZ\} \subset L_0 \subset \text{su}(4)$ rather than within the Weyl chamber, since projecting it onto the Weyl chamber can always be easily performed [15]. It is important to remember that at any given time t the choice of the steering parameters is *not* unique. Therefore, additional requirements (such as smoothness, initial conditions, etc.) must be imposed on the corresponding functions in order to determine the experimentally meaningful trajectory.

Differentiating (11) with respect to the time t gives:

$$\begin{aligned} \frac{dU(t)}{dt} = & -[\alpha'X_1 + \beta'X_2 + c_1'XX + e^{-\alpha X_1}e^{-\beta X_2}(c_2'YY + c_3'ZZ)e^{\beta X_2}e^{\alpha X_1} \\ & + e^{-\alpha X_1}e^{-\beta X_2}e^{-c_2 YY}e^{-c_3 ZZ}(\zeta'X_1 + \xi'X_2)e^{c_3 ZZ}e^{c_2 YY}e^{\beta X_2}e^{\alpha X_1}]U(t). \end{aligned} \quad (12)$$

Here, each of the nested similarity transformations represents a rotation by some angle in a certain two-dimensional subspace of the Lie algebra L_0 . For instance,

$$\begin{aligned} e^{-c_3 ZZ}X_1e^{c_3 ZZ} &= X_1 \cos c_3 + YZ \sin c_3, \\ e^{-c_2 YY}YZe^{c_2 YY} &= YZ \cos c_2 + X_2 \sin c_2, \\ e^{-\alpha X_1}YZe^{\alpha X_1} &= YZ \cos \alpha + ZZ \sin \alpha, \end{aligned} \quad (13)$$

etc. Using (13) to perform algebraic manipulations in (12) and equating the resulting coefficients of the corresponding generators on the right hand sides of (10) and (12), we get a nonlinear system of seven first-order differential equations

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & C_1 & C_2 \\ 0 & 0 & 1 & 0 & 0 & C_2 & C_1 \\ 0 & 0 & 0 & A_1 & A_2 & -A_3C_3 + A_4C_4 & A_3C_4 - A_4C_3 \\ 0 & 0 & 0 & A_2 & A_1 & A_4C_3 - A_3C_4 & -A_4C_4 + A_3C_3 \\ 0 & 0 & 0 & A_3 & -A_4 & A_1C_3 + A_2C_4 & -A_1C_4 - A_2C_3 \\ 0 & 0 & 0 & A_4 & -A_3 & -A_2C_3 - A_1C_4 & A_2C_4 + A_1C_3 \end{bmatrix}}_M \begin{bmatrix} c_1' \\ \alpha' \\ \beta' \\ c_2' \\ c_3' \\ \zeta' \\ \xi' \end{bmatrix} = \begin{bmatrix} g_{xx} \\ \Omega_{1x} \\ \Omega_{2x} \\ g_{yy} \\ g_{zz} \\ g_{yz} \\ g_{zy} \end{bmatrix}, \quad (14)$$

where the new variables

$$C_1 = \cos c_2 \cos c_3, \quad C_2 = \sin c_2 \sin c_3, \quad C_3 = \cos c_2 \sin c_3, \quad C_4 = \sin c_2 \cos c_3, \quad (15)$$

and

$$A_1 = \cos \alpha \cos \beta, \quad A_2 = \sin \alpha \sin \beta, \quad A_3 = \cos \alpha \sin \beta, \quad A_4 = \sin \alpha \cos \beta, \quad (16)$$

have been introduced. Notice that

$$\det M = \cos^2 c_2 - \cos^2 c_3. \quad (17)$$

For simplicity, we choose

$$c_1(0) = \alpha(0) = \beta(0) = c_2(0) = c_3(0) = \zeta(0) = \xi(0) = 0 \quad (18)$$

to satisfy the initial condition $U(0) = 1$.

The first equation in (14) integrates immediately,

$$c_1(t) = \int_0^t d\tau g_{xx}(\tau), \quad (19)$$

while the remaining system can be inverted to give

$$\begin{bmatrix} \alpha' \\ \beta' \\ c_2' \\ c_3' \\ \zeta' \\ \xi' \end{bmatrix} = \begin{bmatrix} \Omega_{1x} + \frac{g_{yy}(A_3C_{33}+A_4C_{22})-g_{zz}(A_3C_{22}+A_4C_{33})-g_{yz}(A_1C_{33}-A_2C_{22})-g_{zy}(A_1C_{22}-A_2C_{33})}{\det M} \\ \Omega_{2x} + \frac{g_{yy}(A_3C_{22}+A_4C_{33})-g_{zz}(A_3C_{33}+A_4C_{22})-g_{yz}(A_1C_{22}-A_2C_{33})-g_{zy}(A_1C_{33}-A_2C_{22})}{\det M} \\ g_{yy}A_1 + g_{zz}A_2 + g_{yz}A_3 + g_{zy}A_4 \\ g_{yy}A_2 + g_{zz}A_1 - g_{yz}A_4 - g_{zy}A_3 \\ \frac{-g_{yy}(A_3C_3+A_4C_4)+g_{zz}(A_3C_4+A_4C_3)+g_{yz}(A_1C_3-A_2C_4)+g_{zy}(A_1C_4-A_2C_3)}{\det M} \\ \frac{-g_{yy}(A_3C_4+A_4C_3)+g_{zz}(A_3C_3+A_4C_4)+g_{yz}(A_1C_4-A_2C_3)+g_{zy}(A_1C_3-A_2C_4)}{\det M} \end{bmatrix}, \quad (20)$$

where

$$C_{22} = \cos c_2 \sin c_2, \quad C_{33} = \cos c_3 \sin c_3. \quad (21)$$

To make further progress, we impose some restrictions on the form of the steering Hamiltonian.

III. ANISOTROPIC EXCHANGE WITH TRACKING CONTROLS

Tracking [19] refers to steering with control parameters having the same enveloping profile defined by some function $\gamma(t)$. Notice that any time-independent Hamiltonian describes tracking with $\gamma(t) = 1$. Here we are interested in Hamiltonians

$$iH(t) = \gamma(t)[\Omega_1 X_1 + \Omega_2 X_2 + g_1(t)XX + g_2YY + g_3ZZ], \quad (22)$$

where $g_1(t)$ is a function of time and $\Omega_1, \Omega_2, g_2, g_3$ are some constants. [It is possible to choose $g_1(t)$ arbitrarily because XX is central in L_0 .]

A. Solving the tracking control case

Under these conditions,

$$c_1(t) = \int_0^t d\tau \gamma(\tau)g_1(\tau). \quad (23)$$

The remaining steering parameters will be found using the ansatz

$$\alpha(t) = \zeta(t), \quad \beta(t) = \xi(t), \quad (24)$$

or, equivalently,

$$U(t) = e^{-\alpha(t)X_1 - \beta(t)X_2} e^{-c_1(t)XX - c_2(t)YY - c_3(t)ZZ} e^{-\alpha(t)X_1 - \beta(t)X_2}. \quad (25)$$

This ansatz works only for Hamiltonians given in (22). For more general systems, another trick or numerical simulations based on (11) and (20) should be used.

The resulting system is

$$\begin{bmatrix} \alpha' \\ \beta' \\ c_2' \\ c_3' \\ \alpha' \\ \beta' \end{bmatrix} = \gamma \begin{bmatrix} \Omega_1 + \frac{(g_2A_4 - g_3A_3)C_{22} + (g_2A_3 - g_3A_4)C_{33}}{\det M} \\ \Omega_2 + \frac{(g_2A_3 - g_3A_4)C_{22} + (g_2A_4 - g_3A_3)C_{33}}{\det M} \\ g_2A_1 + g_3A_2 \\ g_2A_2 + g_3A_1 \\ \frac{-(g_2A_4 - g_3A_3)C_4 - (g_2A_3 - g_3A_4)C_3}{\det M} \\ \frac{-(g_2A_4 - g_3A_3)C_3 - (g_2A_3 - g_3A_4)C_4}{\det M} \end{bmatrix}. \quad (26)$$

The four equations for α' and β' give

$$\alpha' = \frac{\gamma [\Omega_1(1 + \cos c_2 \cos c_3) - \Omega_2 \sin c_2 \sin c_3]}{(\cos c_2 + \cos c_3)^2}, \quad \beta' = \frac{\gamma [\Omega_2(1 + \cos c_2 \cos c_3) - \Omega_1 \sin c_2 \sin c_3]}{(\cos c_2 + \cos c_3)^2}, \quad (27)$$

which determine $\alpha(t)$ and $\beta(t)$ after $c_2(t)$ and $c_3(t)$ had been found. Also,

$$A_3 = \frac{(\Omega_1 g_3 - \Omega_2 g_2) \sin c_2 - (\Omega_1 g_2 - \Omega_2 g_3) \sin c_3}{(g_2^2 - g_3^2)(\cos c_2 + \cos c_3)}, \quad A_4 = \frac{(\Omega_1 g_3 - \Omega_2 g_2) \sin c_3 - (\Omega_1 g_2 - \Omega_2 g_3) \sin c_2}{(g_2^2 - g_3^2)(\cos c_2 + \cos c_3)}. \quad (28)$$

The equations for c'_2 and c'_3 give

$$(c'_2 \pm c'_3)^2 = \gamma^2 (g_2 \pm g_3)^2 (A_1 \pm A_2)^2. \quad (29)$$

Using

$$(A_1 \pm A_2)^2 = 1 - (A_3 \mp A_4)^2, \quad (30)$$

we get

$$(c'_2 \pm c'_3)^2 = \gamma^2 \left[(g_2 \pm g_3)^2 - \frac{(\Omega_1 \mp \Omega_2)^2 (\sin c_2 \pm \sin c_3)^2}{(\cos c_2 + \cos c_3)^2} \right]. \quad (31)$$

After applying the sum-to-product identities and re-arranging the terms, we arrive at

$$\left(\frac{d}{dt} \sin \left(\frac{c_2(t) \pm c_3(t)}{2} \right) \right)^2 + \left(\frac{\gamma(t)}{2} \sqrt{(g_2 \pm g_3)^2 + (\Omega_1 \mp \Omega_2)^2} \sin \left(\frac{c_2(t) \pm c_3(t)}{2} \right) \right)^2 = \left(\frac{\gamma(t)}{2} (g_2 \pm g_3) \right)^2. \quad (32)$$

By making substitution

$$f_{\pm}(t) := \sin \left(\frac{c_2(t) \pm c_3(t)}{2} \right), \quad (33)$$

we can solve the resulting equation

$$\left(\frac{df_{\pm}(t)}{dt} \right)^2 + \left(\frac{\gamma(t)}{2} \sqrt{(g_2 \pm g_3)^2 + (\Omega_1 \mp \Omega_2)^2} f_{\pm}(t) \right)^2 = \left(\frac{\gamma(t)}{2} (g_2 \pm g_3) \right)^2 \quad (34)$$

by inspection. It is easy to see that

$$f_{\pm}(t) = \frac{g_2 \pm g_3}{\sqrt{(g_2 \pm g_3)^2 + (\Omega_1 \mp \Omega_2)^2}} \sin \left(\frac{\sqrt{(g_2 \pm g_3)^2 + (\Omega_1 \mp \Omega_2)^2}}{2} \int_0^t \gamma(\tau) d\tau \right) \quad (35)$$

solves (34) subject to (18), which together with (23), (25), (27) solves the tracking control case:

$$c_{2,3}(t) = \arcsin(f_+(t)) \pm \arcsin(f_-(t)). \quad (36)$$

B. Controlling the flow on the Weyl chamber

Let us now assume that g_1 is tunable, but otherwise independent of time. Then, given an experimentally realizable tracking mechanism $\gamma(t)$, a point on the Weyl chamber (alternatively, in the full Cartan subalgebra A_C) whose XX coordinate is c_1 can be reached after steering for a time t_1 satisfying

$$\int_0^{t_1} \gamma(\tau) d\tau = \frac{c_1}{g_1}. \quad (37)$$

This reachability condition is necessary, but not sufficient. Since the point is specified by a class vector $\vec{c} = (c_1, c_2, c_3)$, we have yet to determine whether the remaining coordinates $c_{2,3}$ can be realized by adjusting the Rabi frequencies $\Omega_{1,2}$. Here we will restrict our attention only to the points belonging to the XX axis, and thus having $c_{2,3} = 0$. It is easy to see that in this case we must have

$$\Omega_{1,2}^{(c_1,0,0)} = \frac{1}{2} \left[\sqrt{\left(\frac{2\pi n g_1}{c_1} \right)^2 - (g_2 - g_3)^2} \pm \sqrt{\left(\frac{2\pi m g_1}{c_1} \right)^2 - (g_2 + g_3)^2} \right], \quad (38)$$

provided the integers n, m are chosen in such a way as to make the Rabi frequencies real.

We can now write down a general condition under which a coupled qubit system directly generates controlled-NOT class corresponding to $\vec{c} = \pi/2 \times (1, 0, 0)$:

$$\int_0^{t_{\text{CNOT}}} \gamma(\tau) d\tau = \frac{\pi}{2g_1}, \quad \Omega_{1,2}^{\text{CNOT}} = \frac{1}{2} \left[\sqrt{(4ng_1)^2 - (g_2 - g_3)^2} \pm \sqrt{(4mg_1)^2 - (g_2 + g_3)^2} \right]. \quad (39)$$

Other approaches to CNOT gate design have been considered in Refs. [20, 21, 22, 23].

C. Tracking control of Josephson phase qubits

1. Capacitive coupling with rf bias of $\Omega_1 \sigma_1^x$ type

In the rotating wave approximation (RWA) [24] the dynamics of two resonant capacitively coupled phase qubits [20, 25, 26, 27, 28, 29] is described by the Hamiltonian

$$H_1(t) = (\gamma(t)/2)[\Omega_1 \sigma_1^x + g(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)], \quad g > 0. \quad (40)$$

The Rabi term represents the action of an rf bias current applied to one of the qubits. It turns out that keeping just one such local term suffices to generate controlled-NOT logic [18]. The condition $\Omega_2 = g_3 = 0$ gives $f_+(t) = f_-(t)$, which leads to

$$c_1(t) = g \int_0^t \gamma(\tau) d\tau, \quad c_2(t) = 2 \arcsin \left[\frac{1}{\sqrt{1 + (\Omega_1/g)^2}} \sin \left(\frac{g}{2} \sqrt{1 + (\Omega_1/g)^2} \int_0^t \gamma(\tau) d\tau \right) \right], \quad c_3(t) = 0, \quad (41)$$

and

$$\alpha(t) = \Omega_1 \int_0^t d\tau \frac{\gamma}{1 + \cos c_2}, \quad \beta(t) = 0. \quad (42)$$

The time-dependent gate is therefore

$$U(t) = e^{-(i/2)\alpha\sigma_1^x} e^{-(i/2)(c_1\sigma_1^x\sigma_2^x + c_2\sigma_1^y\sigma_2^y)} e^{-(i/2)\alpha\sigma_1^x}, \quad (43)$$

which becomes an element of controlled-NOT class, provided [18]

$$\int_0^{t_{\text{CNOT}}} \gamma(\tau) d\tau = \pi/2g, \quad \Omega_1^{\text{CNOT}} = g\sqrt{(4n)^2 - 1}, \quad (44)$$

with $n = 1, 2, 3, \dots$

We may use Result 1 of Ref. [30] to state the following applicability condition for the RWA:

The solution to the Schrödinger equation with the RWA Hamiltonian (40) approximates the solution with exact H (reduced to computational subspace; see Ref. [18] for details) in the sense that if $\Omega_1/\omega \ll 1$ (weak perturbation) and $\omega = \epsilon$ (resonant condition), then $\|\psi_{\text{RWA}}(t) - \psi_{\text{exact}}(t)\| = O(\Omega_1/\omega)$ whenever $0 \leq t \leq O(\omega/\Omega_1)$. Here, ω is the bias frequency, ϵ is the computational level splitting. For UCSB architectures [31] with qubit coupling $g \sim 10$ GHz and level splitting $\omega \lesssim 100$ MHz, $\Omega_1^{\text{CNOT}}/\omega \sim 10^{-2}$.

For calculations that go beyond the RWA in the context of Josephson phase qubits coupled to nanomechanical resonators see Ref. [32].

2. Inductive coupling with rf bias of $\Omega_1 \sigma_1^x + \Omega_2 \sigma_2^x$ type

For inductively coupled qubits [17, 33, 34, 35, 36, 37, 38, 39] driven by local rf magnetic fluxes the Hamiltonian in the RWA is [18]

$$H_2(t) = (\gamma(t)/2)[\Omega_1 \sigma_1^x + \Omega_2 \sigma_2^x + g(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + k\sigma_1^z \sigma_2^z)], \quad g > 0. \quad (45)$$

Using (36), the steering trajectory is found to be

$$\begin{aligned} c_1(t) &= g \int_0^t \gamma(\tau) d\tau, \\ c_{2,3}(t) &= \arcsin \left[\frac{1+k}{\sqrt{(1+k)^2 + [(\Omega_1 - \Omega_2)/g]^2}} \sin \left(\frac{g}{2} \sqrt{(1+k)^2 + [(\Omega_1 - \Omega_2)/g]^2} \int_0^t \gamma(\tau) d\tau \right) \right] \\ &\quad \pm \arcsin \left[\frac{1-k}{\sqrt{(1-k)^2 + [(\Omega_1 + \Omega_2)/g]^2}} \sin \left(\frac{g}{2} \sqrt{(1-k)^2 + [(\Omega_1 + \Omega_2)/g]^2} \int_0^t \gamma(\tau) d\tau \right) \right], \end{aligned} \quad (46)$$

where

$$U(t) = e^{-(i/2)(\alpha\sigma_1^x + \beta\sigma_2^x)} e^{-(i/2)(c_1\sigma_1^x\sigma_2^x + c_2\sigma_1^y\sigma_2^y + c_3\sigma_1^z\sigma_2^z)} e^{-(i/2)(\alpha\sigma_1^x + \beta\sigma_2^x)}, \quad (47)$$

with α and β calculated from Eq. (27). The CNOT class is generated by setting [19]

$$\int_0^{t_{\text{CNOT}}} \gamma(\tau) d\tau = \frac{\pi}{2g}, \quad \Omega_{1,2}^{\text{CNOT}} = \frac{g}{2} \left[\sqrt{(4n)^2 - (1-k)^2} \pm \sqrt{(4m)^2 - (1+k)^2} \right]. \quad (48)$$

For example, for $g = 1.00$, $k = 0.10$ and $n = m = 1$, the Rabi frequencies are $\Omega_1 = 3.8716$, $\Omega_2 = 0.0258$. The corresponding Weyl chamber steering trajectory for $\gamma(t) = 1$, with parameters measured in units of $\pi/2$, is shown in Figures 1, 2, and 3.

3. Inductive coupling with dc bias of $\Omega_1(\sigma_1^z - \sigma_2^z)$ type

Because of the $(X_1, X_2) \rightarrow (Y_1, Y_2) \rightarrow (Z_1, Z_2)$ “symmetry” mentioned in Sec. I, it is possible to devise an alternative CNOT implementation based on the Hamiltonian for inductively coupled qubits acted upon by dc fluxes:

$$H_3(t) = (\gamma(t)/2)[\Omega_1(\sigma_1^z - \sigma_2^z) + g(k\sigma_1^z\sigma_2^z + \sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y)]. \quad (49)$$

The effect of such bias is to “move” system’s energy levels by equal amounts in opposite directions (the process known as *detuning*). One important feature of this implementation is that for any $|k| < 1/2$ it is always possible to generate controlled-NOT logic by choosing Rabi frequencies $0 < |\Omega_1|/g < 1$. This is important when perturbation is required to be small (see Section V for a more general approach).

We have,

$$c_1(t) = kg \int_0^t \gamma(\tau) d\tau, \quad c_2(t) = c_3(t) = \arcsin \left[\frac{1}{\sqrt{1 + (\Omega_1/g)^2}} \sin \left(g \sqrt{1 + (\Omega_1/g)^2} \int_0^t \gamma(\tau) d\tau \right) \right], \quad (50)$$

and

$$\alpha(t) = -\beta(t) = \frac{\Omega_1}{2} \int_0^t d\tau \frac{\gamma}{\cos^2 c_2}, \quad (51)$$

where the steering parameters $(\alpha, \beta, c_1, c_2, c_3)$ are now associated with the operators (Z_1, Z_2, ZZ, XX, YY) . The time-dependent gate is given by

$$U(t) = e^{-(i/2)\alpha(\sigma_1^z - \sigma_2^z)} e^{-(i/2)(c_1\sigma_1^z\sigma_2^z + c_2(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y))} e^{-(i/2)\alpha(\sigma_1^z - \sigma_2^z)}, \quad (52)$$

which implements CNOT class, provided

$$\int_0^{t_{\text{CNOT}}} \gamma(\tau) d\tau = \pi/(2kg), \quad \Omega_1^{\text{CNOT}} = g\sqrt{(2kn)^2 - 1}, \quad (53)$$

where $(2kn)^2 > 1$. Several examples of this implementation are listed in Table I.

Figures 4, 5 show the steering trajectory for $g = 1.00$, $k = 0.10$, and the Rabi frequency $\Omega_1 = 0.6633$.

TABLE I: Generation of controlled-NOT logic with $\vec{c} = (\pi/2) \times (1, 0, 0)$ using inductively coupled flux qubits subject to symmetric dc detuning $(\Omega_1/2)(\sigma_1^z - \sigma_2^z)$. The Hamiltonian is given in (49). Here, $\gamma(t) = 1$.

k	t_{CNOT} , units of $\pi/2g$	n	Ω_1^{CNOT}/g
0.100	10	6	0.6633
		7	0.9798
		8	1.2490
0.050	20	11	0.4583
		12	0.6633
		13	0.8307
		14	0.9798
		15	1.1180
0.025	40	21	0.3202
		22	0.4583
		23	0.5679
		24	0.6633
		25	0.7500
		26	0.8307
		27	0.9069
		28	0.9798
		29	1.0500

IV. DISCUSSION

We now discuss limitations and possible extensions of the proposed method.

The most significant limitation comes from restricting the local terms to form a *homogeneous* pair (such as, for example, (X_1, X_2)). By adopting such restriction we were able to isolate a special subalgebra L_0 of $\text{su}(4)$, given in Eq. (8), that contains a central element. The fifteen-dimensional problem was then reduced to a nonlinear system of “only” seven first-order differential equations, one of which completely separated from the others. By making a certain ansatz, the analytical solution in the tracking control case has been found.

We can extend this approach to Hamiltonians with arbitrary combinations of Rabi terms, such as (X_1, Y_2) , etc. The dimensionality of the problem would increase, but it would still be possible to write down and solve — most likely, numerically — the corresponding system of differential equations.

For Hamiltonians containing *homogeneous* local terms *with arbitrary time dependence* the following useful ansatz can be identified:

Case 1. For

$$H(t) = (1/2)[\Omega_1(t)\sigma_1^x + g_1(t)\sigma_1^x\sigma_2^x + g_2(t)\sigma_1^y\sigma_2^y], \quad (54)$$

use

$$c_3(t) = 0, \quad \beta(t) = \xi(t) = 0, \quad (55)$$

which corresponds to the Cartan decomposition

$$U(t) = e^{-(i/2)\alpha\sigma_1^x} e^{-(i/2)(c_1\sigma_1^x\sigma_2^x + c_2\sigma_1^y\sigma_2^y)} e^{-(i/2)\zeta\sigma_1^x}. \quad (56)$$

Eq. (20) then reduces to

$$\begin{bmatrix} \alpha' \\ c_2' \\ \zeta' \end{bmatrix} = \begin{bmatrix} \Omega_1 - g_2 \sin \alpha \cos c_2 / \sin c_2 \\ g_2 \cos \alpha \\ g_2 \sin \alpha / \sin c_2 \end{bmatrix}. \quad (57)$$

Case 2. Anisotropic exchange with symmetric detuning. This case generalizes the detuning Hamiltonian considered in Section III C 3 by allowing arbitrary time dependent controls:

$$H(t) = (1/2)[\Omega_1(t)(\sigma_1^z - \sigma_2^z) + g_1(t)\sigma_1^z\sigma_2^z + g_2(t)\sigma_1^x\sigma_2^x + g_3(t)\sigma_1^y\sigma_2^y]. \quad (58)$$

In this case we use

$$\alpha(t) = -\beta(t), \quad \zeta(t) = -\xi(t), \quad (59)$$

or

$$U(t) = e^{-(i/2)\alpha(\sigma_1^x - \sigma_2^z)} e^{-(i/2)(c_1\sigma_1^z\sigma_2^z + c_2\sigma_1^x\sigma_2^x + c_3\sigma_1^y\sigma_2^y)} e^{-(i/2)\zeta(\sigma_1^z - \sigma_2^z)}. \quad (60)$$

Eq. (20) now becomes

$$\begin{bmatrix} \alpha' \\ c_2' \\ c_3' \\ \zeta' \end{bmatrix} = \begin{bmatrix} \Omega_1 - (g_2 + g_3) \cos \alpha \sin \alpha (\cos c_3 \sin c_3 - \sin c_2 \cos c_2) / (\cos^2 c_2 - \cos^2 c_3) \\ g_2 \cos^2 \alpha - g_3 \sin^2 \alpha \\ g_3 \cos^2 \alpha - g_2 \sin^2 \alpha \\ (g_2 + g_3) \cos \alpha \sin \alpha / (\cos c_2 \sin c_3 + \sin c_2 \cos c_3) \end{bmatrix}. \quad (61)$$

Case 3. For systems described by

$$H(t) = (1/2)[\Omega_1(t)\sigma_1^x + \Omega_2(t)\sigma_2^x + g_1(t)\sigma_1^x\sigma_2^x + g_2(t)(\sigma_1^y\sigma_2^y + \sigma_1^z\sigma_2^z)] \quad (62)$$

use

$$c_2(t) = c_3(t), \quad \xi(t) = 0, \quad (63)$$

corresponding to

$$U(t) = e^{-(i/2)(\alpha\sigma_1^x + \beta\sigma_2^x)} e^{-(i/2)[c_1\sigma_1^x\sigma_2^x + c_2(\sigma_1^y\sigma_2^y + \sigma_1^z\sigma_2^z)]} e^{-(i/2)\zeta\sigma_1^x}. \quad (64)$$

Notice that in this case we cannot use Eq. (20) directly because matrix M is not invertible, as can be seen from Eq. (17). Instead, the original system (14) has to be re-written in accordance with the constraints imposed by (63). We then get

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & C_1 \\ 0 & 1 & 0 & C_2 \\ 0 & 0 & A_1 + A_2 & -(A_3 - A_4)C_3 \\ 0 & 0 & A_3 - A_4 & (A_1 + A_2)C_3 \end{bmatrix}}_{M_1} \begin{bmatrix} \alpha' \\ \beta' \\ c_2' \\ \zeta' \end{bmatrix} = \begin{bmatrix} \Omega_1 \\ \Omega_2 \\ g_2 \\ 0 \end{bmatrix}, \quad (65)$$

with the variables defined as before, and

$$\det M_1 = \cos c_2 \sin c_2. \quad (66)$$

The system can now be inverted to give

$$\begin{bmatrix} \alpha' \\ \beta' \\ c_2' \\ \zeta' \end{bmatrix} = \begin{bmatrix} \Omega_1 + g_2(A_3 - A_4) \cos c_2 / \sin c_2 \\ \Omega_2 + g_2(A_3 - A_4) \sin c_2 / \cos c_2 \\ g_2(A_1 + A_2) \\ -g_2(A_3 - A_4) / \cos c_2 \sin c_2 \end{bmatrix}, \quad (67)$$

which can be solved numerically.

V. REDUCING LEAKAGE TO NON-COMPUTATIONAL STATES.

Here we describe two controlled-NOT gate implementations satisfying certain constraints that must be imposed on Josephson phase qubits [31] in order to make leakage to higher-lying (non-computational) states small [40, 41, 42], while maintaining the high efficiency of the gate. The relevant conditions are:

1. Hamiltonian:

$$H(t) = (\gamma(t)/2)[\Omega_{x1}\sigma_1^x + \Omega_{x2}\sigma_2^x + \Omega_{y1}\sigma_1^y + \Omega_{y2}\sigma_2^y + \Omega_{z1}\sigma_1^z + \Omega_{z2}\sigma_2^z + g(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y + k\sigma_1^z\sigma_2^z)]. \quad (68)$$

2. Coupling constants:

$$g > 0, \quad |k| < 0.5. \quad (69)$$

3. Number of H applications:

$$N = 1. \quad (70)$$

4. Rabi frequencies:

$$|\Omega_{xi}|, |\Omega_{yi}|, |\Omega_{zi}| \leq g, \quad i = 1, 2. \quad (71)$$

5. Efficiency:

$$\eta := \frac{2\pi}{g t_{\text{gate}}} \geq 2.5. \quad (72)$$

All these constraints can be satisfied by directly steering toward the target belonging to the CNOT equivalence class with entangling part $U_{\text{ent}}(t_{\text{CNOT}})$ represented by the class vector $\vec{c} = (\pi/2) \times (1, 0, 0)$. The *canonical* CNOT gate can then be made out of $U(t_{\text{CNOT}}) = k_1 U_{\text{ent}}(t_{\text{CNOT}}) k_2$ by performing additional local rotations K_1 and K_2 , as usual.

The two implementations are:

1. Symmetric dc detuning:

In this case the Hamiltonian is

$$H_{\text{sym. dc}}^{(-)}(t) = (\gamma(t)/2)[\Omega_1(\sigma_1^x - \sigma_1^y) + \Omega_2(\sigma_2^x - \sigma_2^y) + \underbrace{\Omega_3(\sigma_1^z - \sigma_2^z)}_{\text{symmetric dc detuning}} + g(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + k\sigma_1^z \sigma_2^z)], \quad (73)$$

or, alternatively,

$$H_{\text{sym. dc}}^{(+)}(t) = (\gamma(t)/2)[\Omega_1(\sigma_1^x + \sigma_1^y) + \Omega_2(\sigma_2^x + \sigma_2^y) + \underbrace{\Omega_3(\sigma_1^z - \sigma_2^z)}_{\text{symmetric dc detuning}} + g(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + k\sigma_1^z \sigma_2^z)], \quad (74)$$

with

$$\Omega_1 \equiv g, \quad (75)$$

where $\gamma(t)$ represents experimentally available tracking control, and the superscript (\pm) refers to the corresponding choice of the x and y Rabi parts. The relevant control parameters have been found numerically and are listed in Table II.

Figures 6 and 7 show the steering trajectory for $g = 1.00$, $k = 0.050$, with Rabi frequencies $\Omega_2 = 0.0133$, $\Omega_3 = 0.7575$.

2. Asymmetric dc detuning:

In this case the Hamiltonian is

$$H_{\text{asym. dc}}^{(-)}(t) = (\gamma(t)/2)[\Omega_1(\sigma_1^x - \sigma_1^y) + \Omega_2(\sigma_2^x - \sigma_2^y) + \underbrace{(\Omega_3\sigma_1^z - \Omega_4\sigma_2^z)}_{\text{asymmetric dc detuning}} + g(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + k\sigma_1^z \sigma_2^z)], \quad (76)$$

or, alternatively,

$$H_{\text{asym. dc}}^{(+)}(t) = (\gamma(t)/2)[\Omega_1(\sigma_1^x + \sigma_1^y) + \Omega_2(\sigma_2^x + \sigma_2^y) + \underbrace{(\Omega_3\sigma_1^z - \Omega_4\sigma_2^z)}_{\text{asymmetric dc detuning}} + g(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + k\sigma_1^z \sigma_2^z)], \quad (77)$$

with

$$\Omega_1 = \Omega_3 \equiv g. \quad (78)$$

The corresponding steering controls are listed in Table III.

VI. CONCLUSION

In summary, we have proposed a self-contained approach to steering on the Weyl chamber and applied it to the case of anisotropic exchange with tracking controls, which was solved analytically. It was shown that if architecture allows for local manipulation of individual qubits, *any exchange interaction can generate CNOT quantum logic*. The results were then used to identify several CNOT gate implementations for superconducting Josephson qubits, including the ones that are capable of suppressing leakage to noncomputational states without significant reduction in the gate's efficiency.

TABLE II: Generation of controlled-NOT logic with $\vec{c} = (\pi/2) \times (1, 0, 0)$ using inductively coupled flux qubits driven by weak local perturbations and subject to symmetric dc detuning $(\Omega_3/2)(\sigma_1^z - \sigma_2^z)$. The Hamiltonian is given in Eq. (73) or (74), where $\Omega_1/g \equiv 1$. Here, $\gamma(t) = 1$.

k	t_{CNOT} , units of $\pi/2g$	Ω_2^{CNOT}/g	Ω_3^{CNOT}/g	η
0.000	1.595776	0.000000	0.755502	2.5066
0.001	1.595775	0.000264	0.755503	2.5066
0.002	1.595774	0.000529	0.755505	2.5066
0.003	1.595772	0.000793	0.755509	2.5066
0.004	1.595769	0.001057	0.755515	2.5066
0.005	1.595765	0.001322	0.755522	2.5066
0.010	1.595731	0.002644	0.755582	2.5067
0.025	1.595496	0.006614	0.756001	2.5071
0.050	1.594657	0.013257	0.757500	2.5084
0.075	1.593263	0.019961	0.760001	2.5106
0.100	1.591321	0.026758	0.763506	2.5136
0.150	1.585843	0.040779	0.773549	2.5223
0.250	1.569080	0.071908	0.806036	2.5493
0.350	1.547002	0.111865	0.856120	2.5856
0.450	1.530753	0.178169	0.927506	2.6131
0.490	1.550430	0.240369	0.966790	2.5799
0.493	1.561200	0.254105	0.971189	2.5621

TABLE III: Generation of controlled-NOT logic with $\vec{c} = (\pi/2) \times (1, 0, 0)$ using inductively coupled flux qubits driven by weak local perturbations and subject to asymmetric dc detuning $(\Omega_3/2)\sigma_1^z - (\Omega_4/2)\sigma_2^z$. The Hamiltonian is given in Eq. (76) or (77), where $\Omega_1/g = \Omega_3/g \equiv 1$. Here, $\gamma(t) = 1$.

k	t_{CNOT} , units of $\pi/2g$	Ω_2^{CNOT}/g	Ω_4^{CNOT}/g	η
0.000	1.553771	0.000000	0.402539	2.5744
0.001	1.553770	0.000179	0.402541	2.5744
0.002	1.553768	0.000358	0.402548	2.5744
0.003	1.553766	0.000537	0.402558	2.5744
0.004	1.553762	0.000715	0.402574	2.5744
0.005	1.553757	0.000894	0.402593	2.5744
0.010	1.553716	0.001789	0.402757	2.5745
0.025	1.553430	0.004475	0.403902	2.5749
0.050	1.552414	0.008974	0.407988	2.5766
0.075	1.550736	0.013523	0.414781	2.5794
0.100	1.548418	0.018150	0.424259	2.5833
0.150	1.541995	0.027780	0.451143	2.5940
0.250	1.523410	0.050016	0.535559	2.6256
0.350	1.501442	0.081649	0.659439	2.6641
0.450	1.488962	0.141937	0.826279	2.6864
0.500	1.515587	0.220268	0.938373	2.6392
0.506	1.539498	0.251771	0.959755	2.5982

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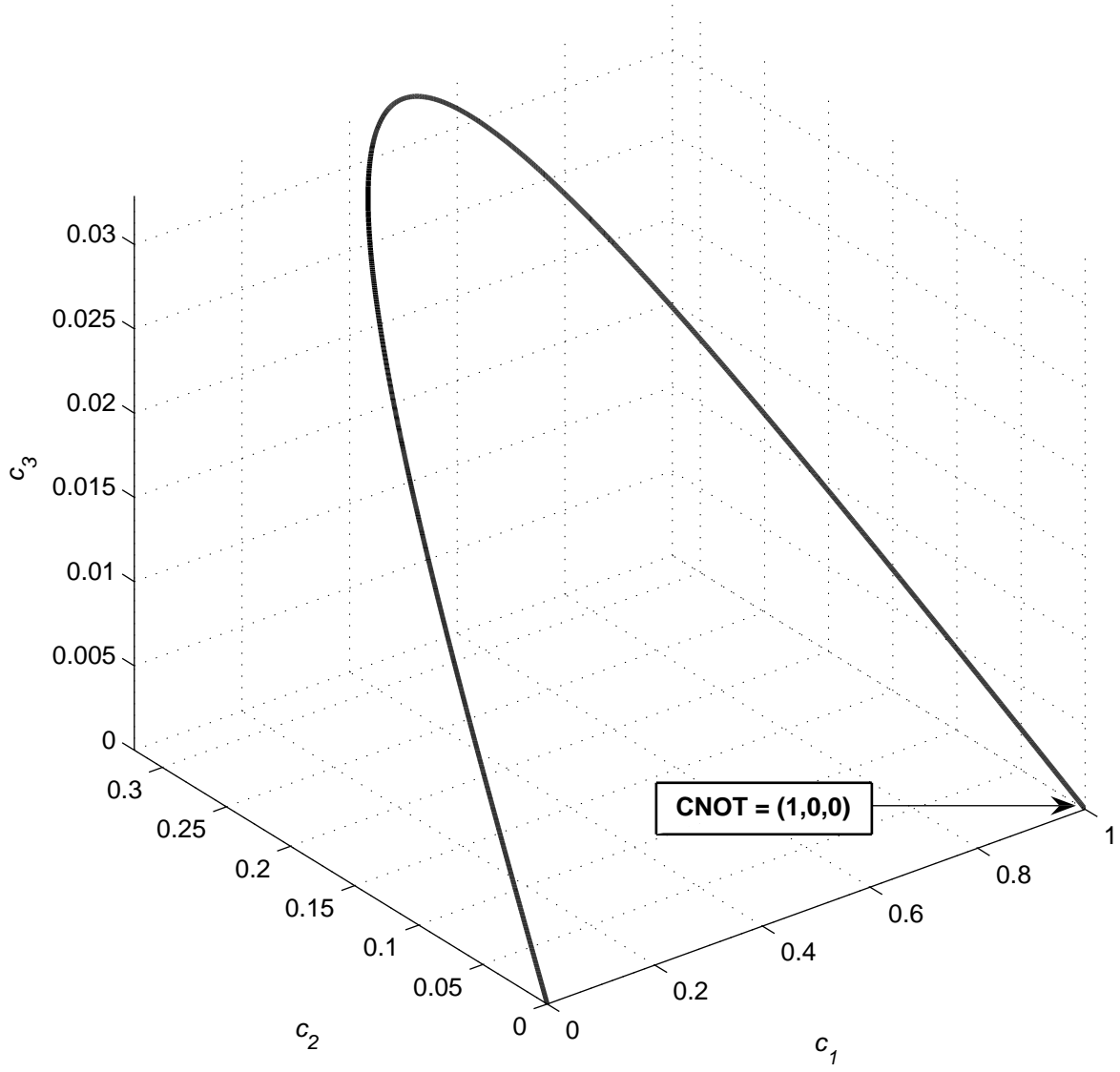


FIG. 1: Steering trajectory generating CNOT class in the case of rf-biased inductively coupled flux qubits, Eq. (45). Here, $g = 1.00$, $k = 0.10$, $\Omega_1 = 3.8716$, $\Omega_2 = 0.0258$, $\gamma(t) = 1$. The steering parameters are given in units of $\pi/2$.

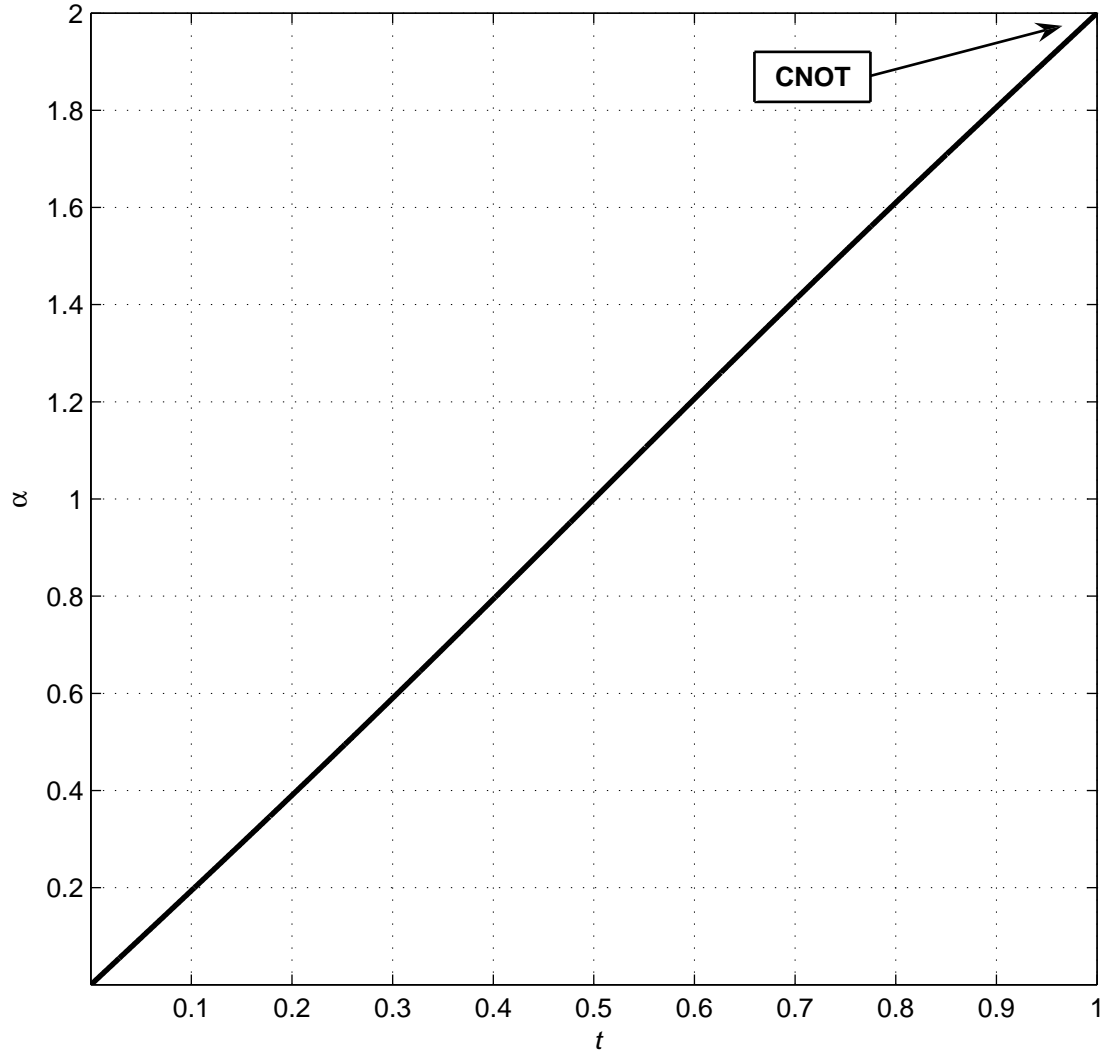


FIG. 2: Local rotation α accompanying the steering trajectory shown in Fig. 1.

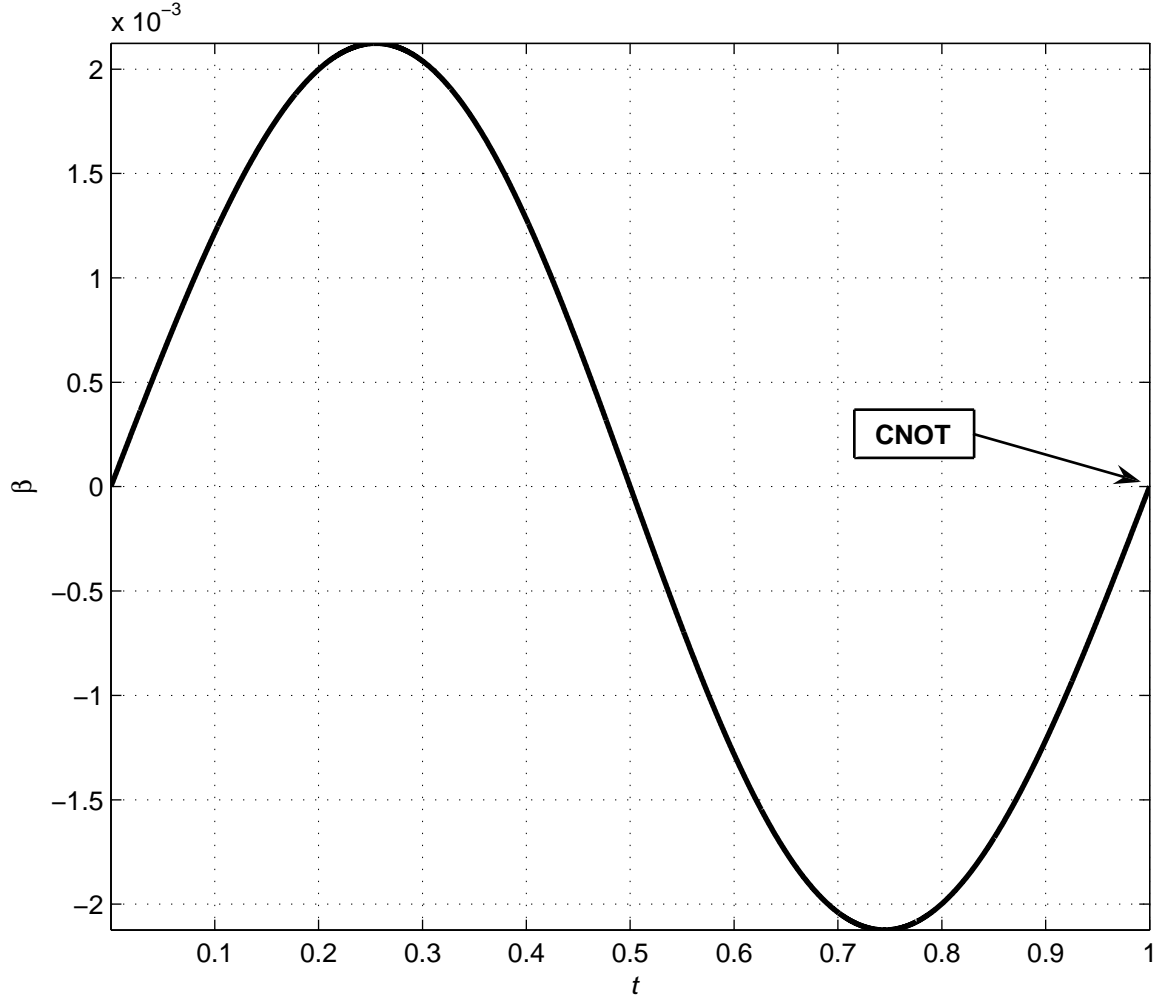


FIG. 3: Local rotation β accompanying the steering trajectory shown in Fig. 1.

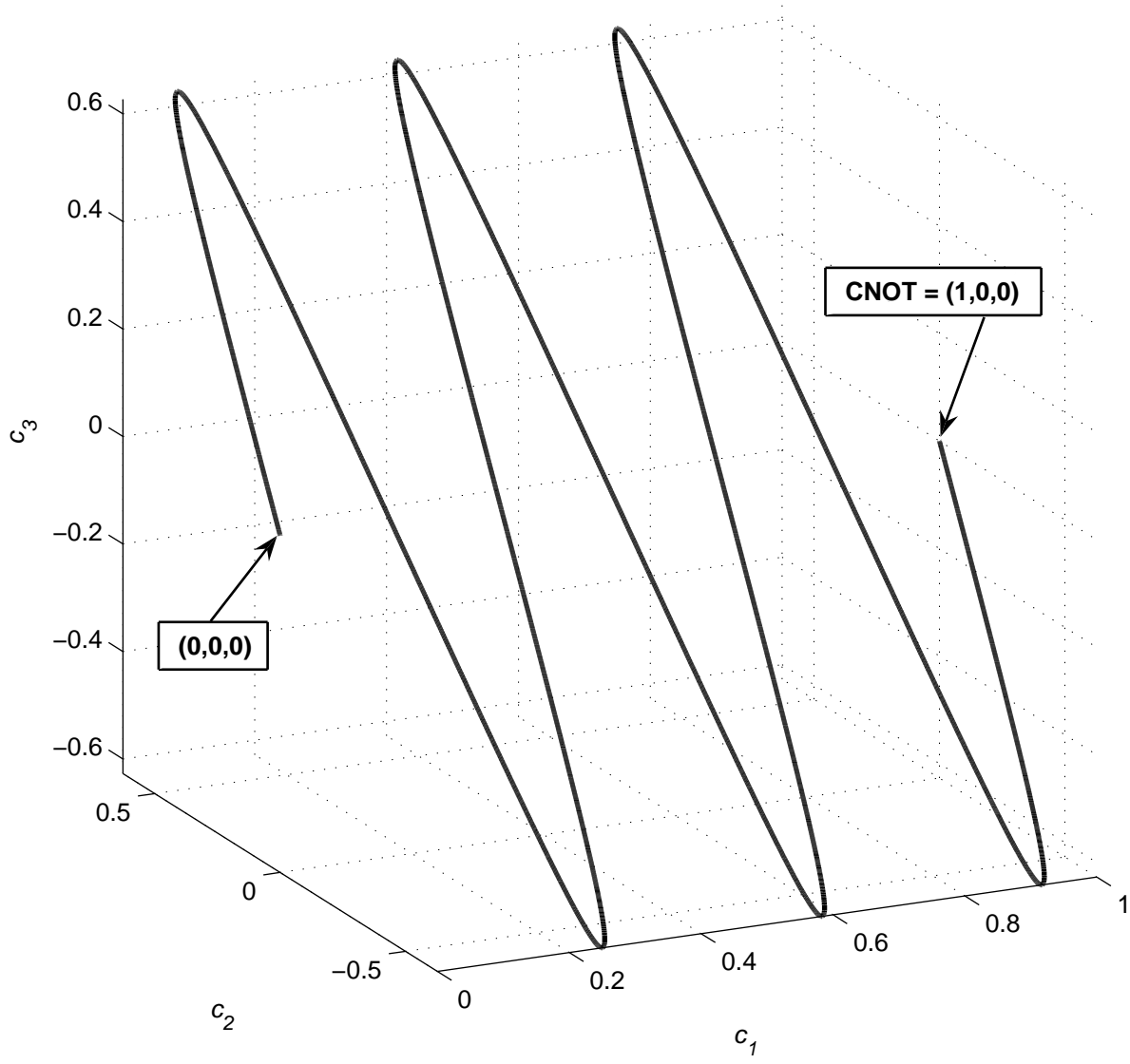


FIG. 4: Steering trajectory generating CNOT class in the case of inductively coupled flux qubits subject to dc symmetric detuning, Eq. (49). Here, $g = 1.00$, $k = 0.10$, $\Omega_1 = 0.6633$, $\gamma(t) = 1$. The steering parameters are given in units of $\pi/2$.

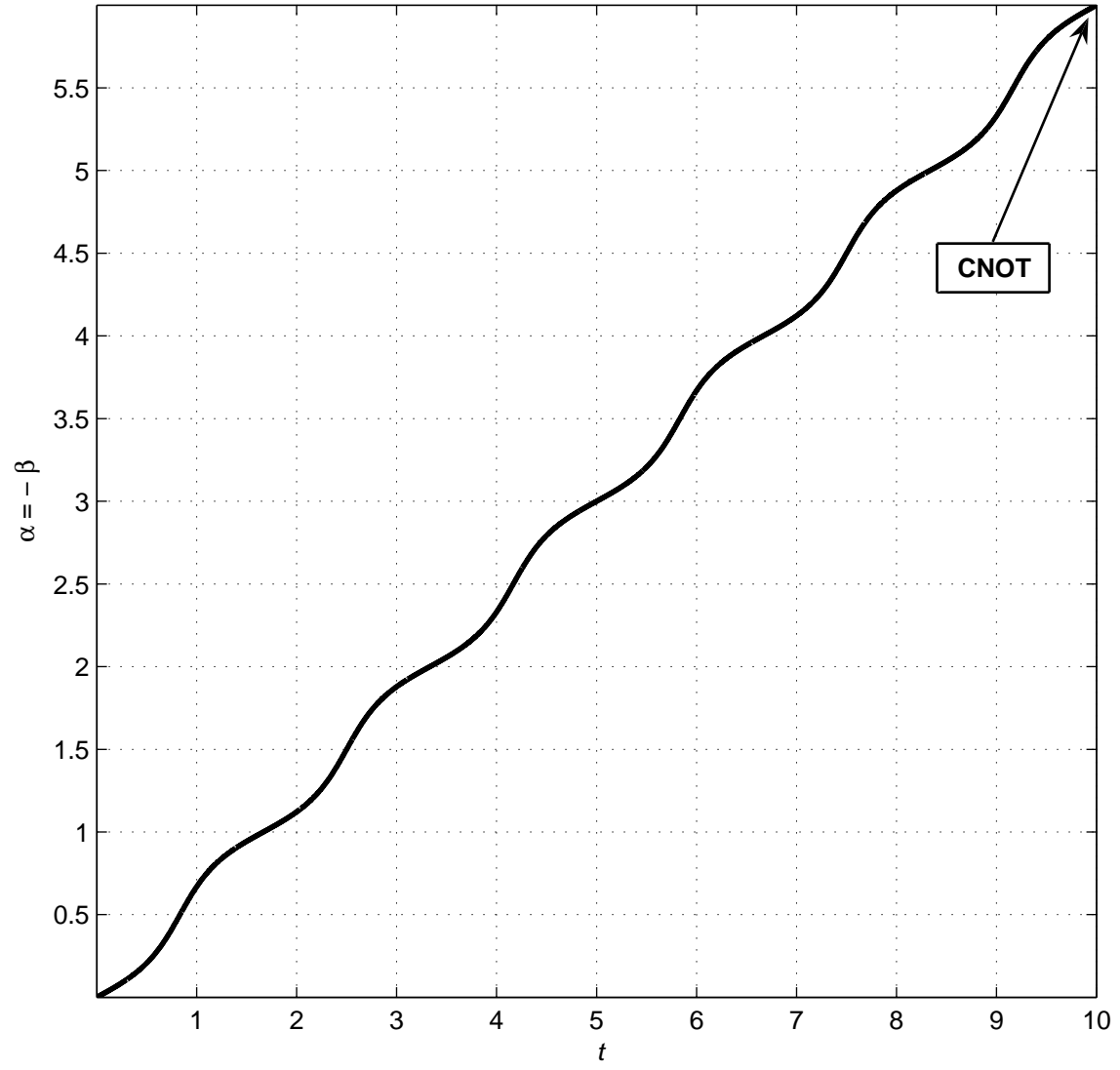


FIG. 5: Local rotations accompanying the steering trajectory shown in Fig. 4.

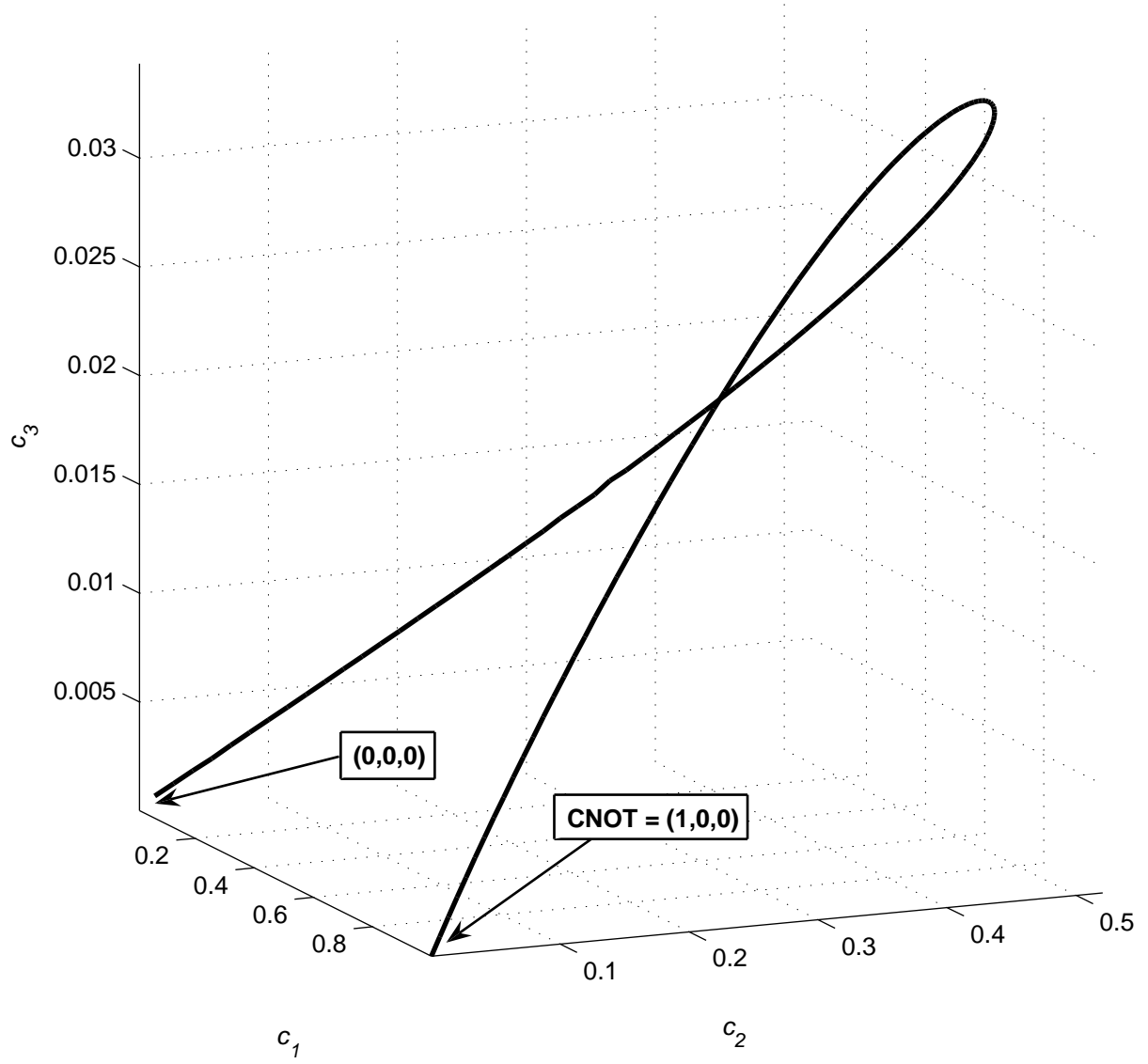


FIG. 6: Weyl chamber steering trajectory generating CNOT class in the case of inductively coupled flux qubits driven by weak local perturbations and subject to symmetric dc detuning, Eq. (73). Here, $g = 1.00$, $k = 0.050$, $\Omega_2 = 0.0133$, $\Omega_3 = 0.7575$, $\gamma(t) = 1$. The steering parameters are given in units of $\pi/2$.

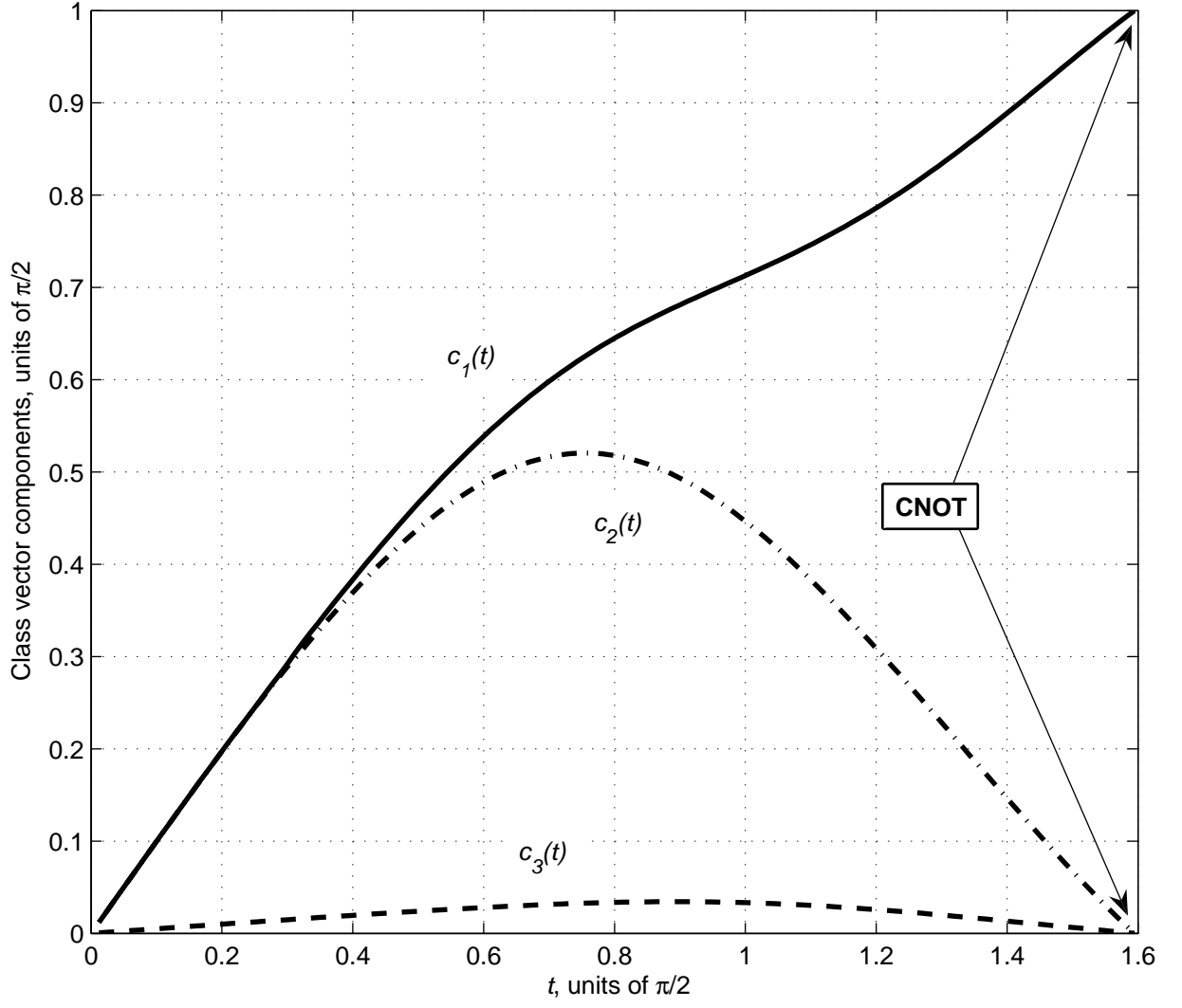


FIG. 7: Time dependence of Weyl chamber steering parameters shown in Fig. 6.